Simulating Recycled Polyethylene Terephthalate-Modified Warm Mix Asphalt

Grant Proposal

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Abstract

The increasing accumulation of polyethylene terephthalate (PET) plastic waste presents a critical environmental challenge, necessitating sustainable reuse strategies. Warm mix asphalt (WMA), produced at lower temperatures than conventional hot mix asphalt, reduces energy consumption and emissions but can suffer from performance limitations such as rutting susceptibility. This study investigates the feasibility of incorporating recycled PET into WMA using a multi-scale simulation approach. Discrete element modeling (DEM) simulations were conducted using YADE to model particle-scale behavior of WMA mixtures containing 0–10% shredded PET as a partial replacement for fine aggregate. Virtual uniaxial compression tests were applied to determine effective modulus and Poisson’s ratio, enabling homogenization of the mixture into representative material properties. These DEM-derived properties were then implemented in finite element modeling (FEM) simulations using Abaqus to evaluate pavement-level mechanical and thermal behavior, including rutting under repeated loading, flexural response, and heat transfer through the asphalt layer. Preliminary DEM results for the control WMA mixture were consistent with published values, validating the modeling framework. FEM simulations indicate that PET-modified WMA is expected to exhibit reduced deformation and slightly improved flexural strength relative to the control mixture. In addition, reduced heat flux was observed, suggesting lower thermal conductivity and improved thermal insulation. Overall, the results suggest that recycled PET can enhance both the mechanical and thermal performance of WMA while supporting sustainability goals through plastic waste recycling. This work establishes a foundation for optimizing PET dosage and demonstrates a transferable simulation framework for evaluating modified asphalt mixtures without extensive physical testing.

Keywords: simulation, discrete element modeling, finite element modeling, warm mix asphalt, polyethylene terephthalate, rutting, flexural strength, thermal conductivity, heat flux

Simulating Recycled Polyethylene Terephthalate-Modified Warm Mix Asphalt

Globally, the annual production of plastics in 2019 was double that of the production in 2000. The trend is predicted to triple by 2060 (United Nations Environment Programme, 2025). These plastics have clogged up landfills and have been a major contributor to pollution. Polyethylene terephthalate (PET) represents a significant amount of this waste, accounting for 60% of all plastics. Being non-biodegradable, the best strategy to stop the environmental effects of PET is through recycling (Usman & Kunlin, 2024). Finding new applications for recycled PET in infrastructure can divert waste PET from landfills.

What is Asphalt?

Asphalt is a composite material widely used in road construction and pavement applications. It is made up of aggregates such as crushed stone, gravel, or sand. These components add strength and durability that are bound together by an asphalt binder: a petroleum-based material that provides the cohesion and flexibility. Chemically, asphalt is a viscoelastic material made mostly of carbon and hydrogen with small amounts of other elements. The binder contains four components which dictate its stiffness, ductility, and flow characteristics (Fernández-Gómez et al., 2013). Asphalt mixtures can be produced using different methods: hot mix asphalt (HMA), warm mix asphalt (WMA), or cold mix asphalt (CMA). These methods differ in temperature and process, and each type has unique advantages when it comes to energy use, performance, and appliance (Jain & Singh, 2021; Kim et al., 2012). For instance, CMA is a cheaper and more environmentally friendly option, but HMA is used more often for high traffic roads due to its increased levels of strength and durability (Jain & Singh, 2021). This study will be based on WMA. WMA is a type of asphalt mixture produced and placed at temperatures 20 – 40 ºC lower than traditional HMA. This temperature reduction is achieved through specialized technologies

Table 1: WMA data compiled from multiple journals from different regions on the reduction in gas emissions when compared to HMA. Table from Rubio et al., 2012.

Emission Type	Vaitkus et al. (2009a,b)	Bueche (2009)	Larsen (2001)	D'Angelo et al. (2009a,b)	Evotherm Website
CO_2	30–40%	30–40%	31%	15–40%	46%
SO_2	35%	–	–	20–35%	81%
VOC	50%	50%	–	>50%	30%
CO	10–30%	–	29%	10–30%	63%
NO_x	60–70%	–	62%	60–70%	58%
Dust	20–25%	–	–	25–55%	–

that temporarily reduce the viscosity of the bitumen binder to improve coating, workability, and compaction. Because less heat is required, WMA production generates fewer gas emissions, consumes less fuel, and creates a safer working environment (Table 1). Research shows that WMA is close to matching the performance of conventional HMA, however challenges like moisture susceptibility and rutting remain (Rubio et al., 2012).

Role of Additives in Asphalt

Adding polymers has been proven to improve certain qualities of the asphalt. For instance, used as a shredded additive to the mortar of stone mastic asphalt (a specific type of HMA), high density polyethylene can improve specific qualities, such as fatigue life, which is the number of stress or strain cycles the asphalt can endure before failing (Figure 2). Waste PET, another example of an additive in stone mastic asphalt, has been found to improve the fatigue properties, as well as increase the fatigue lives or number of stress cycles the asphalt can endure (Moghaddam et al., 2012).

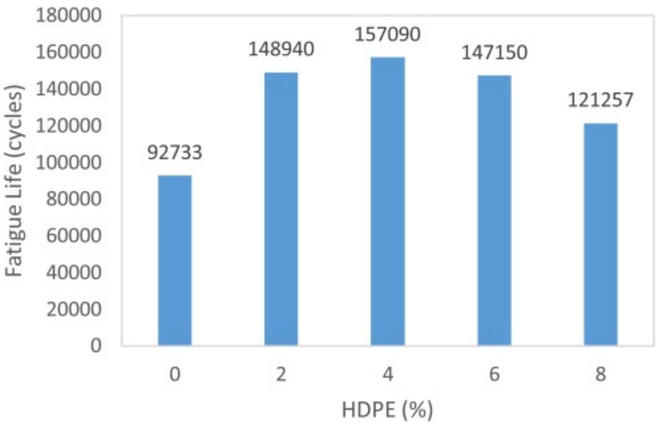


Figure 1: Fatigue Life of SMA Samples Based on HDPE Concentration (Chegenizadeh et al., 2021).

Sustainability and Cost Benefits

Using PET supports sustainable construction by reducing reliance on natural aggregates and minimizing plastic waste. Additionally, PET is more economical, as the asphalt uses recycled materials, which ultimately helps it prevents environmental pollution (Rahmani et al., 2013). Furthermore, PET-modified asphalt has the potential to extend pavement service life, which in turn reduces maintenance and service costs (Usman & Kunlin, 2024).

Knowledge Gaps

WMA has a lack of established ideal ratios for aggregates, bitumen, and additive dosages. This is because most recommendations rely on manufacturer guidelines rather than a standardized criteria. Furthermore, different additives affect WMA differently, creating a need for simulations that can accurately model the behavior of WMA due to its differences from HMA (Rubio et al., 2012).

Discrete Element Modeling

Discrete Element Modeling (DEM) is a simulation method used to analyze the mechanical behavior of mixtures that have many individual particles. The system is represented as many individual particles which have their own movements. The contact between these particles are detected and then their resulting contact forces, characterized by friction and cohesion, are calculated (Cundall & Strack, 1979).

This project utilizes Yet Another Discrete Element (YADE), an open source DEM software. YADE runs on Linux and uses Python. YADE is built on small and replaceable modules that are made up of shapes, contact laws, integrators, engines, and solvers. As such, it is possible to write new contact laws, particle shapes, and engines without modifying the entire codebase (Šmilauer et al., 2021).

Finite Element Modeling

Finite Element Modeling (FEM) is a simulation method used to approximate solutions. It works by dividing a domain into small pieces called finite elements and then solving the equations for these elements. Each of these elements have nodes. Physical fields, such as displacement and temperature, are approximated using shape functions. As such, FEM can solve stress and strain, heat transfer, and more. This means that FEM is used to analyze the stress of beams, analyze fatigue and fracture, and plastic deformation (Jagota et al., 2013). This project utilizes Abaqus, a commercial FEM software developed by Dassault Systèmes (SIMULIA).

Section II: Specific Aims

This proposal aims to evaluate the mechanical performance and feasibility of incorporating recycled polyethylene terephthalate (PET) into warm mix asphalt (WMA) through simulation. The long-term goal is to establish a reliable, low-cost method to divert PET waste from landfills by integrating it into pavement without sacrificing road durability or safety. The hypothesis of this proposal is that the shredded PET will enhance the flexibility, crack resistance, and thermal properties of WMA while also recycling PET. The work proposed will generate data and simulations needed to understand the effect of PET in asphalt and evaluate its practicality in future applications.

Section III: Project Goals and Methodology

Relevance/Significance

Plastic waste, especially PET, continues to increase while current recycling methods are unable to fully prevent it from piling in landfills. Incorporating PET into asphalt offers a reuse option that improves pavement performance while lowering environmental impact. WMA, which is produced at lower temperatures than HMA, further reduces greenhouse gas emissions and energy consumption. Studying PET as a WMA additive is therefore both environmentally and economically significant: it addresses plastic pollution and promotes sustainable construction materials while also improving the performance of asphalt.

Innovation

This project uses DEM and FEM simulations to evaluate PET-modified WMA. While PET has been studied in HMA, its performance in WMA remains understudied. Using both DEM and FEM, the effect of PET in asphalt can be understood at both a particle level and at a pavement level. This can give an indication of the optimal PET dosage without the need for trial-error testing through actual production.

Methodology

First, the DEM software YADE will be used to create virtual WMA samples with varying PET contents. PET will be represented as a separate material with its own specific qualities. The distribution of aggregates in the sample will be 55% coarse and 45% fine, with the qualities of gravel and sand being used. The PET will then serve as a partial replacement of the fine aggregate from 0 to 10% of the total aggregate volume. Then a uniaxial compression and tension test will be applied to create a stress-strain curve that gives the effective modulus of the entire mixture based on the slope. As asphalt is viscoelastic, this is a simplification from the dynamic modulus. Furthermore, Poisson's ratio can be found by measuring the lateral expansion from the axial compression. These values for 0% PET WMA are then compared to literature to make sure there is nothing wrong with the simulation.

After collecting the effective modulus and the Poisson's ratio, the values can be put into Abaqus. In Abaqus, each PET-modified mixture will be modified as a homogenous layer using the DEM values. A pavement section or a simple test specimen can then be created, and the material properties can be assigned to the WMA layer. Cyclic loading will be applied to simulate the effect of vehicle tires or loading, showing the rutting resistance of the WMA. The Abaqus rutting model will allow observation of displacement, showing how PET influences structural performance. Then, a flexural beam model is made to simulate three-point bending. From this, the flexural strength of the WMA can be quantified through stress outputs. Finally, a model will be created in order to simulate the effects of heat transfer; this will used to get values for heat flux. These heat flux values would then be used to calculate the effective thermal conductivity of the WMA.

Specific Aim #1:

Specific Aim #1 is to determine how PET content influences the elastic stiffness of WMA on the particle scale using DEM. The objective is to quantify and compare values from different PET dosages with the control group and understand whether the PET causes the WMA to become stiffer and more resistant to rutting-related deformation at the particle level. The approach is to build DEM specimens of WMA with identical aggregate gradation and binder assumptions; the PET will be used as a partial replacement of the fine aggregate. Then, the specimen will be placed under uniaxial compression in order to calculate for effective modulus and Poisson’s ratio. The rationale is that WMA is not a homogenous mixture; there are smaller and larger rocks randomly distributed throughout the whole block. Since the FEM simulation simulate homogenous mixtures, there is a need to “homogenize” the asphalt. By changing the percentage of PET particles in the DEM simulation, this can be done and lead to accurate FEM simulations.

Justification and Feasibility. The feasibility of using DEM to study the mechanical behavior of asphalt mixtures is supported by De Pue et al. (2019), who successfully calibrated DEM material parameters to reproduce realistic stress-strain curves of unsaturated soils under uniaxial compression (Figure 2). Their results show that DEM can accurately

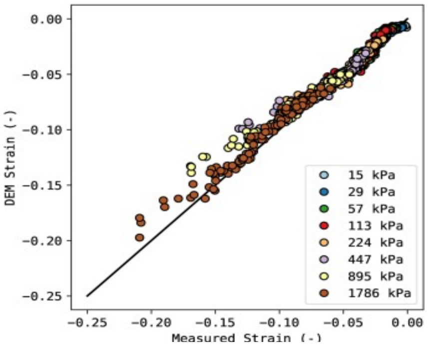


Figure 2: Validation of the stress/strain simulation with calibrated DEM material parameters for 125 samples. RMSE was 6.70 × 10−3 m/m and Pearson r was 0.99 (De Pue et al., 2019).

capture how changes in the parameters of the particles affect the stress-strain relationship of a granular mixture.

This is directly relevant to the current project because PET-modified WMA is also a granular mixture whose behavior depends on the interactions between particles. If DEM is shown to be able to accurately model strain, it can do the same for asphalt if it is given the correct information. As such, the proven ability of DEM to simulate and calibrate stress-strain behavior provides strong justification for its use in determining the effective modulus and Poisson's ratio of PET-modified mixtures in this project.

Summary of Preliminary Data. From the simulation, it was found that the control WMA sample had an effective modulus of 841.838 MPa and a Poisson's ratio of 0.34138, averaged over 5 trials (Table 2). These values fall within the expected range for asphalt mixtures at standard temperatures, supporting the validity of the DEM model. These preliminary findings demonstrate that the DEM framework can replicate the mechanical behavior expected of a warm mix asphalt mixture and produce realistic elastic properties. The consistency across multiple trials shown by the standard error of the mean indicates that the simulation is behaving as intended. Because the DEM calculated properties align with published Poisson's ratio (0.35) and elastic modulus (770 – 911 MPa) for asphalt mixtures at ambient temperatures (Do et al., 2025), these results support the feasibility of using DEM to evaluate how PET content alters mechanical behavior. This provides a strong justification for the approach of DEM software.

Table 2: Recorded Values from DEM Simulation of WMA Control of Effective Modulus and Poisson's Ratio

WMA Control	E Modulus (MPa)	Poisson's Ratio
Trial 1	822.85	0.3348
Trial 2	856.89	0.3486
Trial 3	870.12	0.3562
Trial 4	815.44	0.3217
Trial 5	843.89	0.3456
Average	841.838	0.34138
SEM	10.22	0.0006

Expected Outcomes. The overall outcome of this aim is to create a complete dataset of DEM-made effective modulus and Poisson's ratio for WMA mixtures containing 0-10% PET. This information will reveal whether PET increases stiffness and improves flexibility, as well as serving as inputs for the FEM simulations in Specific Aim #2 and will help determine the optimal PET dosage for structural performance.

Potential Pitfalls and Alternative Strategies. During this specific aim, some potential challenges may arise. First, PET micromechanical parameters such as stiffness, friction, and cohesion are not always well defined in literature, which could introduce uncertainty into the model; to address this, sensitivity analyses will be conducted to identify parameter ranges that reproduce experimentally observed trends. Second, at higher PET contents, the DEM model may generate unrealistic contact behavior or particle interactions. Through adjusting the PET particle size distribution, the simulation should better reflect physical mixtures and remain stable. Finally, DEM simulations are computationally intensive, especially for larger specimens or loading histories. This may need to be changed by reducing specimen size.

Specific Aim #2:

Use FEM in Abaqus to model pavement-level behavior of PET-modified WMA and determine how changes in mixture stiffness influence structural performance. The objective is to quantify the impact of PET-modified mixture stiffness on rutting and flexural strength. The approach is to input the elastic stiffness values derived from the DEM simulation into the FEM model, then simulate realistic loading and boundary conditions to compare the structural responses across different PET contents. The rationale is that FEM can collect stress and displacement values from a load, allowing for an accurate indication of whether PET helps or harms the WMA mixture.

Justification and Feasibility. The feasibility of using finite element modeling (FEM) to evaluate the pavement-level behavior of PET-modified warm mix asphalt is well supported by its established use in simulating asphalt layer responses (Praveen Kumar et al., 2024). Because DEM provides effective modulus and Poisson's ratio values for asphalt mixtures, FEM can use these properties to simulate how changes and interactions between the PET and other aggregates influence the full pavement-layer performance. This is by homogenizing the asphalt into one material. FEM allows for simulating of tensile strain at the bottom of the asphalt layer (flexural strength), compressive strain at the top of the asphalt (rutting), and overall structural response under an average wheel load. By using DEM-derived material properties as FEM inputs, the model can realistically capture how variations in PET content alter pavement performance without requiring full-scale experimental testing.

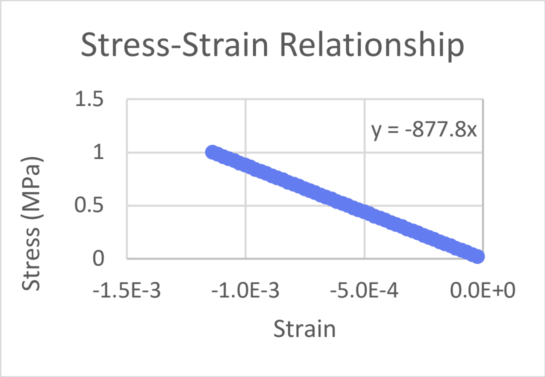


Figure 4: Stress-strain relationship made using displacement and stress from a uniaxial load on the top of the model in FEM

Summary of Preliminary Data. Using Abaqus, three models for mechanical properties were made (see Appendix A). From the simulation of the basic model, a stress-strain relationship was created using displacement and the reaction forces box after being applied with a uniaxial load on the top. This stress-strain relationship was used to make sure that the simulation was working as intended. From this relationship, the slope shows the effective modulus of 877.8 MPa (Figure 4). This value has a 4% error, showing that it is still within a reasonable range. Moreover, this difference in effective modulus is due to the boundary conditions set onto the model that cause it to be slightly stiffer than the DEM model. Given this, the model is assumed to be accurate. Using this model, a simulation was built to show rutting depth through having a moving

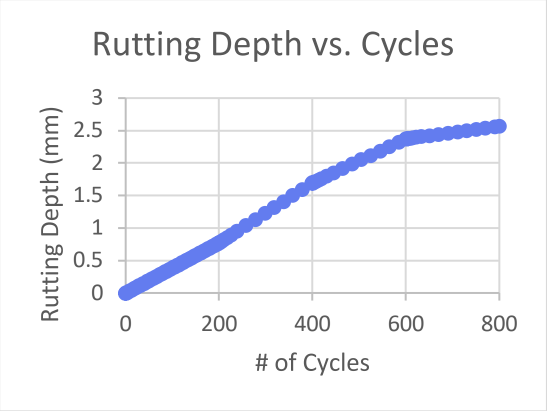


Figure 5: The rutting depth in millimeters plotted with the number of cycles. The maximum rutting depth is around 2.57 mm.

load repeatedly move over the specimen for 800 cycles. After 800 cycles, it was found that the control sample's top layer was about 2.57 mm lower than at the start (Figure 5). Afterwards, a beam model was constructed with the ends being constrained and the center of the top being pressed down on by a load. After a full cycle of the load being placed, it was found that the center dropped down 0.322 mm and had a flexural strength of 1.20546 MPa (Table 3). The values of flexural strength and the graph of rutting depth will be used in order to compare with the PET-modified warm mix asphalt models.

Table 3: Recorded Values From FEM Simulation of WMA Control of Flexural Strength and Midspan Deflection

Midspan Deflection (mm)	Flexural Strength (MPa)
-0.322	1.20546

Expected Outcome. The overall outcome of this aim is to create a usable simulation from FEM for mechanical behavior that utilizes data created from the DEM simulation for WMA mixtures containing 0 to 10% PET. All preliminary data will be used as the control specimen of 0% PET to identify the effects of PET on WMA. This information will reveal whether PET has a positive effect on rutting potential and flexural strength.

Specific Aim #3

Specific Aim #3 is to use FEM in Abaqus to understand the thermal behavior of PET-modified WMA. The objective is to quantify the impact of PET on thermal conductivity. The approach is to modify the original model into including a subgrade layer. Afterwards, the top of the WMA and the bottom of the subgrade will experience a difference in the temperature of 20 ºC. This will allow for comparisons between the heat flux across different PET contents, which can then be used to calculate for effective thermal conductivity using Fourier's Law of Conductivity. The rationale is that FEM can collect thermal behavior from the model, allowing for an accurate indication of whether PET increases or decreases the effective thermal conductivity.

Justification and Feasibility. The feasibility of using FEM simulations to quantify thermal behavior is supported by multiple studies using FEM applications to understand these values. The steady-state method that is used is one of two common methods (Vasanth, 2022). Since FEM uses homogenized material properties, this allows for the heat flux of the specific PET content to be extracted through simulations. This heat flux value can then be used to find thermal conductivity by using the relation found in Fourier's Law of Conductivity.

Summary of Preliminary Data. Using Abaqus, a model for thermal behavior can be created (see Appendix A). From the thermal simulation, the control WMA specimen exhibited a steady-state heat flux magnitude of approximately 199.6 W/m², corresponding to an effective thermal conductivity of 0.998 W/m·K (Table 4). The heat flux increased with applied thermal loading, indicating stable and physically consistent heat transfer behavior across the modeled domain. The resulting thermal conductivity falls within the expected range for asphalt mixtures at ambient conditions, supporting the validity of the FEM thermal framework. These preliminary findings demonstrate that the coupled thermal model can reproduce realistic heat flow responses in warm mix asphalt. Together with the mechanical DEM results, this confirms that the simulation environment is capable of capturing both elastic and thermal behavior of WMA materials. This

Table 4: Recorded Values From FEM Simulation of WMA Control of Heat Flux and the Calculated Thermal Conductivity

Heat Flux (W/m²)	Thermal Conductivity (W/m·K)
199.6	0.998

establishes a reliable baseline for subsequent parametric studies and provides justification for extending the model to investigate how recycled PET content influences thermal conductivity and overall heat transfer performance.

Expected Outcome. The overall outcome of this aim is to create a usable simulation from FEM for thermal behavior that utilizes data created from the DEM simulation for WMA mixtures containing 0 to 10% PET. All preliminary data will be used as the control specimen of 0% PET to identify the effects of PET on WMA. This information will reveal whether PET causes the thermal conductivity to decrease or increase.

Section IV: Resources/Equipment

The proposed research is entirely computational and requires no physical laboratory facilities. Simulations will be conducted using standard computing hardware with YADE for discrete element modeling and the Abaqus Student Edition for finite element analysis. Data processing and visualization will be performed in Excel, with published literature guiding model calibration and validation. The use of widely available software makes the project cost-effective and feasible within the scope of this grant.

Section V: Ethical Considerations

As a computational study, the primary ethical considerations relate to research integrity, responsible data usage, and proper attribution of sources. All software used in this project will be accessed and utilized in accordance with applicable licensing agreements. Open-source tools will be cited appropriately, and any published data used for validation or comparison will be referenced accurately. Results will be reported honestly and without exaggeration. Additionally, this project aligns with ethical principles of environmental responsibility by exploring sustainable engineering solutions that reduce plastic waste and promote resource reuse. Overall, the proposed work adheres to accepted ethical standards for computational engineering research.

Section VI: Timeline

November

- Installed and learned DEM (YADE) and FEM (Abaqus) software.
- Began building initial simulation models.

Late November-Early December

- Developed the baseline DEM model for control WMA.
- Extracted elastic properties and validated results against literature.
- Built baseline FEM models and confirmed realistic mechanical behavior.

December

- Expanded FEM models to simulate rutting and flexural response.
- Established reusable mechanical simulation frameworks.

January

- Added thermal modeling to study heat transfer through asphalt layers.
- Modified DEM models to incorporate multiple PET contents.
- Ran parametric simulations and compiled mechanical and thermal outputs.

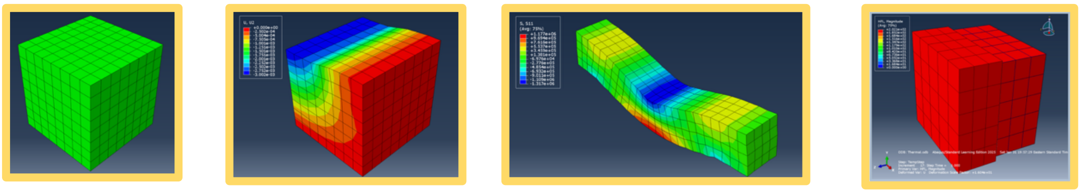
Late January-Early February

- Integrated PET-dependent properties into FEM.
- Compared control and PET-modified mixtures.
- Organized results for stiffness, deformation, flexural behavior, and thermal performance.

Section VII: Appendix

Appendix A

Abaqus Simulation Models



1. 2. 3. 4.

Models made using Abaqus software. 1. Basic cubic model for stress-strain response (0.1 m x 0.1 m x 0.1 m). 2. Visualization and model of rutting depth simulation. Rutting depth simulation showing vertical displacement contours, where blue indicates greater negative displacement (0.1 m x 0.1 m x 0.1 m). 3. Flexural strength simulation showing stress contours, where blue indicates compressive stress and red indicates tensile stress (0.3 m x 0.05 m x 0.05 m). 4. FEM heat flux magnitude contours in the WMA model under steady-state thermal loading. Heat flux outputs were extracted to calculate effective thermal conductivity using Fourier's law. (0.1 m x 0.1 m x 0.1 m).

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